

LOW DENSITY LIMIT OF BCS THEORY AND BOSE-EINSTEIN CONDENSATION OF FERMION PAIRS

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ABSTRACT. We consider the low density limit of a Fermi gas in the BCS approximation. We show that if the interaction potential allows for a two-particle bound state, the system at zero temperature is well approximated by the Gross-Pitaevskii functional, describing a Bose-Einstein condensate of fermion pairs.

1. INTRODUCTION AND MAIN RESULTS

1.1. Introduction. The bosonic behavior of pairs of fermions is a topic that has been investigated in condensed matter physics for more than half a century. It plays a crucial role in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [2], and is used to explain the superfluid behavior of He^3 and cold gases of fermionic atoms, for instance. As long as the pair of fermions is tightly bound, it is not surprising that it effectively behaves like a boson, and hence can form a Bose-Einstein condensate (BEC). In BCS theory the pairing mechanism is also important under very weak attraction where the separation of the paired particles can be much larger than the average particle spacing, however.

It was realized in the eighties [14, 15] that BCS theory actually applies both to the case of BECs of tightly bound fermions and to cases where the pairing mechanism is very weak. The regime in-between is called the BEC-BCS crossover regime [18, 4]. This crossover is currently a hot topic in condensed matter physics, and recent experiments on cold atomic gases have been able to probe large parts of this regime. We refer to [3] for a recent review.

From the mathematical physics point of view, the pairing mechanism in fermionic systems is poorly understood, and there are no rigorous results starting from first principle, i.e., with an appropriate many-body Hamiltonian. In this work, we shall *assume* the BCS approximation to be correct, and investigate some of its consequences. This paper can be viewed as a sequel to the recent work [6, 7] where the emergence of Ginzburg-Landau (GL) theory [8] from BCS theory was studied. Close to the critical temperature, GL arises as an effective theory on the macroscopic scale, describing the variations in the density of fermion pairs. For this it is not necessary to form actual bound states between the fermions, a very weak attraction is sufficient for pairing.

In this paper we are interested in the low density limit in the case where the inter-particle interaction *does* allow for two-particle bound states. We consider the system at zero temperature and show that the macroscopic variations in the pair density are, to leading order, correctly described by the Gross-Pitaevskii (GP) functional [9, 17],

describing a BEC of fermion pairs with an effective *repulsive* interaction. We allow for a large class of possible interactions among the particles. Essentially our sole assumption will be the existence of two-particle bound states. The existence of such bound states is crucial here. In their absence one obtains an ideal Fermi gas in the low density limit, up to exponentially small corrections [5, 12, 13].

The proof of our results uses the same tools as the proof of the main theorem in [6]. Parts of it are simpler, in fact, since we work at zero temperature here. We shall demonstrate that the semiclassical estimates in [6] extend to the zero temperature case.

1.2. The BCS Functional. We consider a macroscopic sample of a system of spin $1/2$ fermions at zero temperature. For simplicity, we restrict our attention to three spatial dimensions, but our analysis applies to any dimension $1 \leq d \leq 3$. The interaction among the fermions is described by a local two-body potential V . In addition, the particles are subject to external electric and/or magnetic fields. Neutral atoms would not couple to these fields, of course, but there can be other forces, e.g., arising from rotation, with a similar mathematical description. In BCS theory the state of the system is described in terms of a 2×2 operator valued matrix

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1 - \bar{\gamma} \end{pmatrix} \quad (1.1)$$

satisfying $0 \leq \Gamma \leq 1$ as an operator on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. The bar denotes complex conjugation, i.e., $\bar{\alpha}$ has the integral kernel $\overline{\alpha(x, y)}$. The fact that Γ is hermitian implies that γ is hermitian and α is symmetric, i.e., $\gamma(x, y) = \overline{\gamma(y, x)}$ and $\alpha(x, y) = \alpha(y, x)$. Moreover, since $\Gamma^2 \leq \Gamma$, we have $0 \leq \gamma \leq 1$ and $0 \leq \alpha \bar{\alpha} \leq \gamma(1 - \gamma)$.

We are interested in the effect of weak and slowly varying external fields. Hence we introduce a small parameter $h > 0$ and write the external magnetic and electric potentials as $hA(hx)$ and $h^2W(hx)$, respectively. In order to avoid having to introduce boundary conditions, we assume that the system is infinite and periodic with period h^{-1} , in all three directions. In particular, A and W are periodic, and we assume that the state Γ is periodic. Our goal is to calculate the ground state energy per unit volume, and the corresponding BCS minimizer.

We find it convenient to do a rescaling and use macroscopic variables instead of the microscopic ones. The rescaled BCS functional has the form

$$\begin{aligned} \mathcal{E}^{\text{BCS}}(\Gamma) := & \text{Tr} \left[\left((-ih\nabla + hA(x))^2 - \mu + h^2W(x) \right) \gamma \right] \\ & + \int_{\mathcal{C} \times \mathbb{R}^3} V(h^{-1}(x - y)) |\alpha(x, y)|^2 dx dy \end{aligned} \quad (1.2)$$

where \mathcal{C} denotes the unit cube $[0, 1]^3$, and Tr stands for the trace per unit volume. Explicitly, if χ denotes the characteristic function of \mathcal{C} , and B is a periodic operator with $\chi B \chi$ trace class, $\text{Tr } B$ equals the usual trace of $\chi B \chi$. The location of the cube is obviously of no importance. Using the Floquet decomposition [19, Sect. XIII.16], it is not difficult to see that the trace per unit volume has the usual properties of a trace like cyclicity, for instance, and standard inequalities like Hölder's inequality hold. This is discussed in detail in [6, Sect. 3].

In (1.2) we choose units such that the particle mass equals 1. The particles have spin $1/2$, which adds an extra factor 2 to the energy. The chemical potential is denoted by $\mu/2$, for convenience, and the external electric potential is really $W/2$.

For heuristic arguments explaining the derivation of the BCS functional (1.2), we refer to [10, Appendix A]. The BCS state of the system is a minimizer of this functional over all admissible states Γ , i.e., periodic Γ of the form (1.1) satisfying $0 \leq \Gamma \leq 1$.

We make the following assumptions on the potentials A and W in (1.2). Our results presumably hold under slightly weaker regularity assumptions on W and A , but to keep things simple we shall not aim for the weakest possible conditions.

Assumption 1. *We assume both W and A to be periodic with period 1. We further assume that $\widehat{W}(p)$ and $|\widehat{A}(p)|(1 + |p|)$ are summable, with $\widehat{W}(p)$ and $\widehat{A}(p)$ denoting the Fourier coefficients of W and A , respectively. In particular, $W \in C^0(\mathbb{R}^3)$ and $A \in C^1(\mathbb{R}^3)$.*

The interaction potential will be assumed to satisfy the following properties.

Assumption 2. *The interaction potential V is assumed to be real-valued and reflection-symmetric, i.e., $V(x) = V(-x)$, with $V \in L^{3/2}(\mathbb{R}^3)$. Moreover, the Schrödinger operator $-\nabla^2 + V(x)$ has a negative energy bound state.*

The $L^{3/2}$ assumption on V guarantees relative form-boundedness with respect to the Laplacian. The ground state energy of $-\nabla^2 + V(x)$ will be denoted by $-E_b < 0$, and its ground state wave function by α_0 . It is unique up to a phase factor. We find it convenient to normalize α_0 such that

$$\int_{\mathbb{R}^3} |\widehat{\alpha}_0(q)|^2 \frac{dq}{(2\pi)^3} = 1, \quad (1.3)$$

with $\widehat{\alpha}_0(q) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \alpha(x) e^{-iq \cdot x} dx$ denoting the Fourier transform.

In the following, we are interested in the case $\mu = -E_b + h^2 \delta\mu$, which corresponds to the low density limit. We find it convenient to absorb the constant $h^2 \delta\mu$ into the potential W , i.e., we set $\mu = -E_b$ and write $W(x)$ instead of $W(x) - \delta\mu$.

1.3. The GP Functional. Let $\psi \in H_{\text{per}}^1(\mathbb{R}^3)$, the periodic functions in $H_{\text{loc}}^1(\mathbb{R}^3)$. For $g \geq 0$, the GP functional is defined as

$$\mathcal{E}^{\text{GP}}(\psi) = \int_{\mathbb{C}} \left[\frac{1}{4} |(-i\nabla + 2A(x))\psi(x)|^2 + W(x)|\psi(x)|^2 + g|\psi(x)|^4 \right] dx. \quad (1.4)$$

The coefficient 2 in front of the vector potential A is due to the fact that ψ describes pairs of particles, and the charge of a pair is twice the particle charge. The factor 4 in front of the kinetic energy is twice the mass of a fermion pair. The coefficient g will be calculated below from BCS theory.

We denote the ground state energy of the GP functional by

$$E^{\text{GP}}(g) = \inf \{ \mathcal{E}(\psi) : \psi \in H_{\text{per}}^1(\mathbb{R}^3) \}. \quad (1.5)$$

It is not difficult to show that under our assumptions on A and W , there exists a corresponding minimizer, which satisfies a second order differential equation known as the GP equation. Note that there is no normalization constraint on ψ , the normalization is determined by the chemical potential which is contained in $W(x)$.

1.4. Main Results. We define the energy $E^{\text{BCS}}(\mu)$ as the infimum of \mathcal{E}^{BCS} over all admissible Γ , i.e.,

$$E^{\text{BCS}}(\mu) = \inf_{\Gamma} \mathcal{E}^{\text{BCS}}(\Gamma). \quad (1.6)$$

Recall that a state Γ is admissible if $0 \leq \Gamma \leq 1$ and Γ is periodic, i.e., it commutes with translations by 1 in the three coordinate directions.

Recall also that α_0 denote the ground state of $-\nabla^2 + V(x)$, normalized as in (1.3).

THEOREM 1. *Let*

$$g = \int_{\mathbb{R}^3} |\hat{\alpha}_0(q)|^4 (q^2 + E_b) \frac{dq}{(2\pi)^3}. \quad (1.7)$$

Under Assumptions 1 and 2 above, we have, for small h ,

$$E^{\text{BCS}}(-E_b) = h (E^{\text{GP}}(g) + e), \quad (1.8)$$

with e satisfying the bounds $\text{const } h \geq e \geq -\text{const } h^{1/5}$. Moreover, if Γ is an approximate minimizer of \mathcal{E}^{BCS} at $\mu = -E_b$, in the sense that $\mathcal{E}^{\text{BCS}}(\Gamma) \leq h(E^{\text{GP}}(g) + \epsilon)$ for some small $\epsilon > 0$, then the corresponding α can be decomposed as

$$\alpha = \frac{h}{2} (\psi(x) \hat{\alpha}_0(-ih\nabla) + \hat{\alpha}_0(-ih\nabla) \psi(x)) + \sigma \quad (1.9)$$

with $\mathcal{E}^{\text{GP}}(\psi) \leq E^{\text{GP}}(g) + \epsilon + \text{const } h^{1/5}$ and

$$\int_{\mathcal{C} \times \mathbb{R}^3} |\sigma(x, y)|^2 dx dy \leq \text{const } h^{3/5}. \quad (1.10)$$

To appreciate the bound (1.10), note that the square of the $L^2(\mathcal{C} \times \mathbb{R}^3)$ norm of the first term on the right side of (1.9) is of the order h^{-1} , and hence is much larger than the one of σ . To leading order in h , the pair wave function $\alpha(x, y)$ is thus given by

$$\frac{\psi(x) + \psi(y)}{2(2\pi)^{3/2} h^2} \alpha_0(h^{-1}(x - y)), \quad (1.11)$$

with ψ a minimizer of the GP functional (1.4). This agrees with

$$\frac{\psi(\frac{1}{2}(x + y))}{(2\pi)^{3/2} h^2} \alpha_0(h^{-1}(x - y)) \quad (1.12)$$

to leading order in h , hence ψ describes the center of mass motion of pairs of fermion with are bound in the ground state of $-h^2 \nabla^2 + V(x/h)$.

Note that g in (1.7) is strictly positive, even for purely attractive interaction potentials V . In the limit of a point interaction [1, Sect. I.1] with scattering length $a_s > 0$ we have

$$\hat{\alpha}_0(q) = \frac{\sqrt{8\pi} E_b^{1/4}}{q^2 + E_b} \quad \text{and} \quad E_b = \frac{1}{a_s^2}, \quad (1.13)$$

and hence $g = 2\pi a_s$. Since the mass of the fermion pairs is 2, this corresponds to a scattering length of $2a_s$ for the pair scattering [20]. The factor 2 is an artifact of the BCS approximation; an investigation of the actual four-body problem with pseudo-potentials predicts a scattering length $\approx 0.6 a_s$ [16].

By varying the external potential W , our bounds (1.8) on the ground state energy can be used to obtain bounds on the particle density as well. In particular, the number of particles per unit volume, N , can be calculated by replacing $W(x)$ by $W(x) + \delta\mu$

and taking the derivative of the energy with respect to $\frac{1}{2}h^2\delta\mu$ at $\delta\mu = 0$. To leading order in h , the result is that

$$N = \frac{2}{h} \int_{\mathcal{C}} |\psi^{\text{GP}}(x)|^2 dx \quad (1.14)$$

where ψ^{GP} is a minimizer of the GP functional (1.4). The average particle density, in microscopic variables, is $\rho = h^3 N = 2h^2 \int |\psi^{\text{GP}}|^2$ and is thus of order h^2 . Hence our scaling limit corresponds indeed to low density.

In the translation invariant case, where $A(x) = 0$ and $W(x) = -\delta\mu < 0$ is constant, the GP minimizer is given by $|\psi^{\text{GP}}(x)|^2 = \delta\mu/(2g)$, and $E^{\text{GP}}(g) = -\delta\mu^2/(4g)$. In particular, the ground state energy per particle, which is equal to $E^{\text{BCS}}(\mu)/N + \frac{1}{2}\mu$, is given by

$$-\frac{1}{2}E_{\text{b}} + \frac{1}{2}g\rho + \text{higher order in } \rho \quad (1.15)$$

for small density ρ .

1.5. Outline of the paper. In the following Section 2 we shall state our main semiclassical estimates. These are a crucial input to obtain the bounds in Theorem 1. They are an extension to zero temperature of the analogous expressions at positive temperature obtained in [6, Sect. 2]. An upper bound on E^{BCS} will be derived in Section 3, using the variational principle. Finally, Section 4 contains the lower bound. In this final section also the structure of approximate minimizers will be investigated. This leads to a definition of the order parameter ψ . Our proof follows closely the proof of the main theorem in [6], but is partly simpler due to the fact that we work at zero temperature.

Throughout the proofs, C will denote various different constants. We will sometimes be sloppy and use C also for expressions that depend only on some fixed, h -independent, quantities like E_{b} or $\|W\|_{\infty}$, for instance.

2. SEMICLASSICAL ESTIMATES

This section contains the semiclassical estimates needed in the proof of Theorem 1. Let ψ be a periodic function in $H_{\text{loc}}^2(\mathbb{R}^3)$. Pick a reflection-symmetric and real-valued function t , with the property that

$$\partial^{\gamma} t \in L^6(\mathbb{R}^3) \quad (2.1)$$

and

$$\int_{\mathbb{R}^3} \frac{|\partial^{\gamma} t(q)|^2}{1+q^2} dq < \infty \quad (2.2)$$

for all multi-indices $\gamma \in \{0, 1, \dots, 4\}^3$. We shall later choose $t(q) = 2(q^2 + E_{\text{b}})\hat{\alpha}_0(q)$, but the results of this section are valid for general functions t satisfying (2.1) and (2.2).

Let Δ denote the periodic operator

$$\Delta = -\frac{h}{2} (\psi(x)t(-ih\nabla) + t(-ih\nabla)\psi(x)) , \quad (2.3)$$

and let

$$H_\Delta = \begin{pmatrix} (-ih\nabla + hA(x))^2 - \mu + h^2W(x) & \Delta \\ \bar{\Delta} & -(ih\nabla + hA(x))^2 + \mu - h^2W(x) \end{pmatrix} \quad (2.4)$$

on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, with A and W satisfying Assumption 1. We shall also assume that $\mu < 0$. In the following, we will investigate the trace per unit volume of the negative part of H_Δ . Specifically, we are interested in the effect of the off-diagonal term Δ in H_Δ , in the semiclassical regime of small h .

THEOREM 2. *Let $[s]_- = \frac{1}{2}(|s| - s)$ denote the negative part. For $\mu < 0$, the diagonal entries of the 2×2 matrix-valued operator $[H_\Delta]_- - [H_0]_-$ are locally trace class, and the sum of their traces per unit volume (which will be denoted by Tr_0) equals*

$$\begin{aligned} \text{Tr}_0([H_\Delta]_- - [H_0]_-) &= -h^{-1}E_1 - hE_2 + O(h^2) \left(\|\psi\|_{H^1(C)}^4 + \|\psi\|_{H^1(C)}^2 \right) \\ &\quad + O(h^3) \left(\|\psi\|_{H^1(C)}^6 + \|\psi\|_{H^2(C)}^2 \right), \end{aligned} \quad (2.5)$$

where

$$E_1 = -\frac{1}{2}\|\psi\|_2^2 \int_{\mathbb{R}^3} \frac{t(q)^2}{q^2 - \mu} \frac{dq}{(2\pi)^3} \quad (2.6)$$

and

$$\begin{aligned} E_2 &= -\frac{1}{8} \sum_{j,k=1}^3 \langle \partial_j \psi | \partial_k \psi \rangle \int_{\mathbb{R}^3} t(q) [\partial_j \partial_k t](q) \frac{1}{q^2 - \mu} \frac{dq}{(2\pi)^3} \\ &\quad + \left(\frac{1}{8} \|(\nabla + 2iA)\psi\|_2^2 + \frac{1}{2} \langle \psi | W | \psi \rangle \right) \int_{\mathbb{R}^3} \frac{t(q)^2}{(q^2 - \mu)^2} \frac{dq}{(2\pi)^3} \\ &\quad + \frac{1}{8} \|\psi\|_4^4 \int_{\mathbb{R}^3} \frac{t(q)^4}{(q^2 - \mu)^3} \frac{dq}{(2\pi)^3}. \end{aligned} \quad (2.7)$$

The error terms in (2.5) of order h^2 and h^3 depend on t only via bounds on the expressions (2.1) and (2.2), and are uniform in μ for $\mu < 0$ bounded away from zero.

Here, we use the short-hand notation $\|\psi\|_p$ for the norm on $L^p(\mathcal{C})$. Likewise, $\langle \cdot | \cdot \rangle$ denotes the inner product on $L^2(\mathcal{C})$.

In general, the operator $[H_\Delta]_- - [H_0]_-$ is not trace class under our assumptions on t and ψ . Hence the trace in (2.5) has to be suitably understood as the sum of the traces of the diagonal entries. This issue is further discussed in the next section.

The proof of Theorem 2 is very similar to the proof of Theorem 2 in [6]. In the following, we shall limit ourselves to explaining the main differences.

Sketch of proof. Since $\mu < 0$ and $W(x)$ and $\psi(x)t(-ih\nabla)$ are bounded, both H_Δ and H_0 have, for small enough h , a gap around 0 in the spectrum. Hence the projector onto the negative spectral subspace can be written via a contour integral as

$$\theta(-H_\Delta) = \frac{1}{2\pi i} \int_{\ell} \frac{1}{z - H_\Delta} dz, \quad (2.8)$$

where $\theta(t) = 1$ for $t \geq 1$ and 0 otherwise, and ℓ is the contour $\{r - i, r \in (-\infty, 0]\} \cup \{ir, r \in [-1, 1]\} \cup \{-r + i, r \in [0, \infty)\}$. The integral has to be understood as a suitable

weak limit over finite contours. Similarly, one obtains that

$$[H_0]_- - [H_\Delta]_- = \frac{1}{2\pi i} \int_\ell z \left(\frac{1}{z - H_\Delta} - \frac{1}{z - H_0} \right) dz. \quad (2.9)$$

The remaining analysis proceeds as in [6, Sect. 8] (compare with Eq. (8.11) there), and we shall not repeat it here. In [6], the factor z on the right side of (2.9) is replaced by $-\beta^{-1} \ln(1 + e^{-\beta z})$ and the contour is around the whole real axis. For $\beta \rightarrow \infty$, this reduces to (2.9), given the gap in the spectrum around 0. \square

Our second semiclassical estimate concerns the upper off-diagonal term of the projection onto the negative spectral subspace of H_Δ , $\theta(-H_\Delta)$, which we denote by α_Δ . We are interested in its H^1 norm. In general, we define the H^1 norm of a periodic operator O by

$$\|O\|_{H^1}^2 = \text{Tr} \left[O^\dagger (1 - h^2 \nabla^2) O \right]. \quad (2.10)$$

In other words, $\|O\|_{H^1}^2 = \|O\|_2^2 + h^2 \|\nabla O\|_2^2$. Note that this definition is not symmetric, i.e., $\|O\|_{H^1} \neq \|O^\dagger\|_{H^1}$ in general.

THEOREM 3. *Let $\varphi(q) = \frac{1}{2}t(q)/(q^2 - \mu)$. Under the same assumptions as in Theorem 2, we have*

$$\left\| \alpha_\Delta - \frac{h}{2} (\psi(x)\varphi(-ih\nabla) + \varphi(-ih\nabla)\psi(x)) \right\|_{H^1} \leq Ch^{3/2} \left(\|\psi\|_{H^2(\mathcal{C})} + \|\psi\|_{H^1(\mathcal{C})}^3 \right). \quad (2.11)$$

The proof follows again along the same lines as the proof of the corresponding Theorem 3 in [6], and we shall only sketch the differences.

Sketch of proof. With the aid of (2.8) we can write

$$\alpha_\Delta = \frac{1}{2\pi i} \int_\ell \left[\frac{1}{z - H_\Delta} \right]_{12} dz, \quad (2.12)$$

where $[\cdot]_{ij}$ stands for the ij element of an operator-valued matrix, and where the integral has to be suitably understood as a weak limit, similarly to (2.9). Alternatively, one could integrate over $-\ell$, since the identity operator has vanishing off-diagonal terms.

Using the resolvent identity and the definitions of Δ and φ we find that

$$\alpha_\Delta = \frac{h}{2} (\psi(x)\varphi(-ih\nabla) + \varphi(-ih\nabla)\psi(x)) + \sum_{j=1}^3 \eta_j, \quad (2.13)$$

where

$$\eta_1 = \frac{h}{4\pi i} \int_\ell \left(\frac{1}{z - k_0} [\psi, k_0] \frac{t}{z^2 - k_0^2} + \frac{t}{z^2 - k_0^2} [\psi, k_0] \frac{1}{z + k_0} \right) dz, \quad (2.14)$$

$$\eta_2 = \frac{1}{2\pi i} \int_\ell \frac{1}{z - k_0} \left((k - k_0) \frac{1}{z - k} \Delta + \Delta \frac{1}{z + k_0} (k_0 - k) \right) \frac{1}{z + k} dz \quad (2.15)$$

and

$$\eta_3 = \frac{1}{2\pi i} \int_\ell \frac{1}{z - k} \Delta \frac{1}{z + k} \Delta^\dagger \frac{1}{z - k} \Delta \left[\frac{1}{z - H_\Delta} \right]_{22} dz. \quad (2.16)$$

Here, t is short for the operator $t(-ih\nabla)$, $k = (-ih\nabla + hA(x))^2 - \mu + h^2W(x)$ and $k_0 = -h^2\nabla^2 - \mu$.

Proceeding as in [6, Section 9] one sees that

$$\|\eta_1\|_{H^1} \leq Ch^{3/2}\|\psi\|_{H^2(\mathcal{C})}, \quad (2.17)$$

$$\|\eta_2\|_{H^1} \leq Ch^{3/2}\|\psi\|_{H^1(\mathcal{C})} \quad (2.18)$$

and

$$\|\eta_3\|_{H^1} \leq Ch^{3/2}\|\psi\|_{H^1(\mathcal{C})}^3. \quad (2.19)$$

In the terms investigated in [6], there is an additional factor $(1+e^{\beta z})^{-1}$ in the integrand, and the contour contains the whole real axis. Similarly as in the proof of Theorem 2, this reduces to our case as $\beta \rightarrow \infty$. \square

3. PROOF OF THEOREM 1: UPPER BOUND

Recall that α_0 denotes the unique ground state of $-\nabla^2 + V(x)$, normalized as in (1.3). It satisfies $\alpha_0(x) = \alpha_0(-x)$, and we can take it to be real. In the following, we let t denote the Fourier transform of $2(-\nabla^2 + E_b)\alpha_0 = -2V\alpha_0$, i.e.,

$$t(q) = -2(2\pi)^{-3/2} \int_{\mathbb{R}^3} V(x)\alpha_0(x)e^{-iq \cdot x} dx = 2(q^2 + E_b)\hat{\alpha}_0(q). \quad (3.1)$$

It satisfies all the assumptions in the previous section. In particular, (2.1) and (2.2) hold for all $\gamma \in \mathbb{N}_0^3$. This can be shown, for instance, in the same way as in [6, Sect. 4]. The method there also implies that $\sqrt{|V(x)|}\alpha_0(x)e^{\kappa|x|} \in L^2(\mathbb{R}^3)$ for $\kappa < E_b^{1/2}$, and that $\int_{\mathbb{R}^3} (|x^\gamma \nabla \alpha_0(x)|^2 + |x^\gamma \alpha_0(x)|^2) dx < \infty$ for all $\gamma \in \mathbb{N}_0^3$. Some of these properties will be used later on.

As a trial state, we use

$$\Gamma_\Delta = \begin{pmatrix} \gamma_\Delta & \alpha_\Delta \\ \bar{\alpha}_\Delta & 1 - \bar{\gamma}_\Delta \end{pmatrix} = \theta(-H_\Delta) \quad (3.2)$$

where H_Δ is given in (2.4) with Δ as in (2.3) and $\mu = -E_b$. For t , we choose (3.1), which is reflection symmetric and can be taken to be real.

We have

$$[H_0]_- - [H_\Delta]_- = H_\Delta \Gamma_\Delta - H_0 \Gamma_0 = \begin{pmatrix} k\gamma_\Delta + \Delta\bar{\alpha}_\Delta & k\alpha_\Delta + \Delta(1 - \bar{\gamma}_\Delta) \\ \bar{\Delta}\gamma_\Delta + \bar{k}\bar{\alpha}_\Delta & \bar{k}\bar{\gamma}_\Delta + \bar{\Delta}\alpha_\Delta \end{pmatrix} \quad (3.3)$$

where k denotes the upper left entry of H_Δ (and H_0). From (1.2) and (3.3) we conclude that

$$\begin{aligned} \mathcal{E}^{\text{BCS}}(\Gamma_\Delta) &= -\frac{1}{2} \text{Tr}_0 ([H_\Delta]_- - [H_0]_-) \\ &\quad - h^{-4} \int_{\mathcal{C} \times \mathbb{R}^3} V\left(\frac{x-y}{h}\right) \left| \frac{1}{2}(\psi(x) + \psi(y))\alpha_0\left(\frac{x-y}{h}\right) \right|^2 \frac{dx dy}{(2\pi)^3} \\ &\quad + \int_{\mathcal{C} \times \mathbb{R}^3} V\left(\frac{x-y}{h}\right) \left| \frac{\psi(x) + \psi(y)}{2h^2(2\pi)^{3/2}} \alpha_0\left(\frac{x-y}{h}\right) - \alpha_\Delta(x, y) \right|^2 dx dy, \end{aligned} \quad (3.4)$$

where Tr_0 stands for the sum of the traces per unit volume of the diagonal entries of the 2×2 matrix-valued operator. In general, the operator $[H_0]_- - [H_\Delta]_-$ is not trace

class if Δ is not, as can be seen from (3.3). In the evaluation of $\mathcal{E}^{\text{BCS}}(\Gamma_\Delta)$ only the diagonal terms of (3.3) enter, however.

The first term on the right side of (3.4) was calculated in Theorem 2 above. Note that, for our choice of t , the integral in the second term in (2.7) is equal to 4, and the integral in the third term is $16g$.

As in [6, Sect. 5] we can rewrite the second term on the right side of (3.4) as

$$\begin{aligned} & -h^{-4} \int_{\mathbb{R}^3 \times \mathcal{C}} V(h^{-1}(x-y)) \left| \frac{1}{2}(\psi(x) + \psi(y))\alpha_0(h^{-1}(x-y)) \right|^2 dx dy \\ &= \frac{1}{16h} \sum_{p \in (2\pi\mathbb{Z})^3} |\widehat{\psi}(p)|^2 \int_{\mathbb{R}^3} \frac{t(q)}{q^2 + E_b} (2t(q) + t(q-hp) + t(q+hp)) dq. \end{aligned} \quad (3.5)$$

Using the Taylor expansion

$$\begin{aligned} & 2t(q) + t(q-hp) + t(q+hp) \\ &= 4t(q) + h^2 [(p \cdot \nabla)^2 t](q) + \frac{h^4}{6} \int_{-1}^1 [(p \cdot \nabla)^4 t](q + shp)(1-|s|)^3 ds \end{aligned} \quad (3.6)$$

we see that (3.5) equals

$$\frac{\|\psi\|_2^2}{4h} \int_{\mathbb{R}^3} \frac{t(q)^2}{q^2 + E_b} dq + \frac{h}{16} \sum_{i,j=1}^3 \langle \partial_i \psi | \partial_j \psi \rangle \int_{\mathbb{R}^3} t(q) [\partial_i \partial_j t](q) \frac{1}{q^2 + E_b} dq + O(h^3), \quad (3.7)$$

where the error term is bounded by

$$Ch^3 \|\psi\|_{H^2}^2 \int_{\mathbb{R}^3} |V(x)| |\alpha_0(x)|^2 |x|^4 dx. \quad (3.8)$$

Note that the first term in (3.7) cancels the contribution of $h^{-1}E_1$ in (2.6) to the trace $\frac{1}{2} \text{Tr}([H_\Delta]_- - [H_0]_-)$.

It remains to investigate the last term in (3.4). Since V is relatively bounded with respect to the Laplacian, we can bound the term by an appropriate H^1 norm. Recall the definition of the H^1 norm of a periodic operator in (2.10). For general periodic operators O , we have the bound

$$\left| \int_{\mathcal{C} \times \mathbb{R}^3} V\left(\frac{x-y}{h}\right) |O(x,y)|^2 dx dy \right| \leq \left\| (1 - \nabla^2)^{-1/2} V(\cdot) (1 - \nabla^2)^{-1/2} \right\| \|O\|_{H^1}^2. \quad (3.9)$$

The operator of relevance here is given by

$$O = \alpha_\Delta - \frac{h}{2} (\psi(x) \widehat{\alpha}_0(-ih\nabla) + \widehat{\alpha}_0(-ih\nabla) \psi(x)). \quad (3.10)$$

Note that, for our choice of t , we have $\varphi(q) = \frac{1}{2}t(q)/(q^2 + E_b) = \widehat{\alpha}_0(q)$. Hence Theorem 3 implies that the H^1 norm of (3.10) is bounded by $Ch^{3/2}(\|\psi\|_{H^2} + \|\psi\|_{H^1}^3)$.

For ψ , we shall take a minimizer of the GP functional (1.4). Under Assumption 1 on W and A , it is easily seen to be in H^2 . Collecting all the terms, we see that for this choice of ψ we have

$$E^{\text{BCS}}(-E_b) \leq \mathcal{E}^{\text{BCS}}(\Gamma_\Delta) \leq h(E^{\text{GP}} + Ch) \quad (3.11)$$

for small h . This completes the proof of the upper bound.

4. PROOF OF THEOREM 1: LOWER BOUND

Our proof of the lower bound on $E^{\text{BCS}}(-E_b)$ in Theorem 1 consists of two main parts. The goal of this first part is to show the following.

Proposition 1. *Let Γ be a state satisfying $\mathcal{E}^{\text{BCS}}(\Gamma) \leq 0$, and let α denote its off-diagonal element. Then there exists a periodic function ψ , with $H^1(\mathcal{C})$ norm bounded independently of h , such that*

$$\alpha = \frac{h}{2}(\psi(x)\hat{\alpha}_0(-ih\nabla) + \hat{\alpha}_0(-ih\nabla)\psi(x)) + \xi \quad (4.1)$$

with $\|\xi\|_{H^1} \leq O(h^{1/2})$ for small h .

Recall the definition (2.10) for the H^1 norm of a periodic operator. The bound $\|\xi\|_{H^1} \leq O(h^{1/2})$ has to be compared with the H^1 norm of the first part of (4.1), which is $O(h^{-1/2})$ (for fixed $\psi \neq 0$.)

Proof. Let $K^{A,W}$ denote the operator

$$K^{A,W} = (-ih\nabla + hA(x))^2 + E_b + h^2W(x), \quad (4.2)$$

and $\lambda^{A,W} = \inf \text{spec } K^{A,W} \geq E_b - O(h^2)$. For all admissible states Γ , we have

$$0 \leq \alpha\bar{\alpha} \leq \gamma(1 - \gamma) \leq \gamma \quad (4.3)$$

and hence

$$\begin{aligned} \text{Tr } K^{A,W} \gamma &\geq \text{Tr } K^{A,W} (\alpha\bar{\alpha} + \gamma^2) \geq \text{Tr } K^{A,W} \alpha\bar{\alpha} + \lambda^{A,W} \text{Tr } \gamma^2 \\ &\geq \text{Tr } K^{A,W} \alpha\bar{\alpha} + \lambda^{A,W} \text{Tr } (\alpha\bar{\alpha})^2. \end{aligned} \quad (4.4)$$

In particular,

$$\mathcal{E}^{\text{BCS}}(\Gamma) \geq \lambda^{A,W} \text{Tr } (\alpha\bar{\alpha})^2 + \int_{\mathcal{C}} \langle \alpha(\cdot, y) | K^{A,W} + V(h^{-1}(\cdot - y)) | \alpha(\cdot, y) \rangle dy. \quad (4.5)$$

Here $K^{A,W}$ acts on the x variable of $\alpha(x, y)$, and $\langle \cdot | \cdot \rangle$ denotes the standard inner product on $L^2(\mathbb{R}^3)$.

By definition, the operator $K^{0,0} + V(h^{-1}(\cdot - y))$ on $L^2(\mathbb{R}^3)$ has a unique ground state $h^{-3/2}\alpha_0(h^{-1}(x - y))$, with ground state energy zero, and a gap above. To utilize this fact, it will be convenient to replace $K^{A,W}$ by $K^{0,0}$ in (4.5). We claim that

$$K^{A,W} + V(h^{-1}(\cdot - y)) \geq \frac{1}{2} (K^{0,0} + V(h^{-1}(\cdot - y))) - h^2 (\|W\|_{\infty} + \|A\|_{\infty}^2). \quad (4.6)$$

This follows immediately from the fact that

$$\begin{aligned} K^{A,W} + V(h^{-1}(\cdot - y)) &= \frac{1}{2} (K^{0,0} + V(h^{-1}(\cdot - y))) \\ &\quad + \frac{1}{2} (K^{2A,0} + V(h^{-1}(\cdot - y))) - h^2 A(x)^2 + h^2 W(x) \end{aligned} \quad (4.7)$$

and that $K^{2A,0} + V(h^{-1}(\cdot - y)) \geq 0$, by the diamagnetic inequality.

For any state Γ with $\mathcal{E}^{\text{BCS}}(\Gamma) \leq 0$ we conclude from (4.5) and (4.6) that

$$\lambda^{A,W} \text{Tr } (\alpha\bar{\alpha})^2 + \frac{1}{2} \int_{\mathcal{C}} \langle \alpha(\cdot, y) | K^{0,0} + V(h^{-1}(\cdot - y)) | \alpha(\cdot, y) \rangle dy \leq Ch^2 \|\alpha\|_2^2. \quad (4.8)$$

To show that this inequality implies (4.1), we shall proceed as in [6, Sect. 6].

Define ψ to be the periodic function

$$\psi(y) = \frac{1}{(2\pi)^{3/2}h} \int_{\mathbb{R}^3} \alpha_0(h^{-1}(x-y))\alpha(x,y) dx. \quad (4.9)$$

If we write

$$\alpha(x,y) = \frac{1}{(2\pi)^{3/2}h^2} \alpha_0(h^{-1}(x-y))\psi(y) + \xi_0(x,y) \quad (4.10)$$

the gap in the spectrum of $K^{0,0} + V(h^{-1}(\cdot - y))$ above zero, together with (4.8) and the normalization (1.3), yields the bound $\|\xi_0\|_2 \leq O(h)\|\alpha\|_2$. We can also symmetrize and write

$$\alpha(x,y) = \frac{\psi(x) + \psi(y)}{2(2\pi)^{3/2}h^2} \alpha_0(h^{-1}(x-y)) + \xi(x,y), \quad (4.11)$$

again with $\|\xi\|_2 \leq O(h)\|\alpha\|_2$. In order to complete the proof of (4.1), we need to show that $\|\psi\|_{H^1}$ is bounded independently of h , and that the H^1 norm of ξ is bounded by $O(h^{1/2})$.

An application of Schwarz's inequality yields

$$\int_{\mathcal{C}} |\psi(x)|^2 dx \leq h\|\alpha\|_2^2 \leq \int_{\mathcal{C}} |\psi(x)|^2 dx + h\|\xi_0\|_2^2. \quad (4.12)$$

Since $\|\xi_0\|_2 \leq O(h)\|\alpha\|_2$, this implies that

$$\|\alpha\|_2^2 \leq (1 + O(h^2)) \frac{1}{h} \int_{\mathcal{C}} |\psi(x)|^2 dx. \quad (4.13)$$

Again by using Schwarz's inequality,

$$\int_{\mathcal{C}} |\nabla \psi(x)|^2 dx \leq \frac{1}{h} \int_{\mathbb{R}^3 \times \mathcal{C}} |(\nabla_x + \nabla_y) \alpha(x,y)|^2 dx dy. \quad (4.14)$$

The latter expression can be bounded as

$$\int_{\mathbb{R}^3 \times \mathcal{C}} |(\nabla_x + \nabla_y) \alpha(x,y)|^2 dx dy \leq \frac{4}{h^2} \int_{\mathcal{C}} \langle \alpha(\cdot, y) | K^{0,0} + V(\frac{\cdot - y}{h}) | \alpha(\cdot, y) \rangle dy. \quad (4.15)$$

To see this, expand $\alpha(x,y)$ in a Fourier series

$$\alpha(x,y) = \sum_{p \in (2\pi\mathbb{Z})^3} e^{ip \cdot (x+y)/2} \tilde{\alpha}_p(x-y). \quad (4.16)$$

Using that $\tilde{\alpha}_p(x) = \tilde{\alpha}_p(-x)$ for all $p \in (2\pi\mathbb{Z})^3$ we see that (4.15) is equivalent to

$$K^{\frac{1}{2}p,0} + K^{-\frac{1}{2}p,0} + 2V(x/h) \geq \frac{1}{2}h^2p^2. \quad (4.17)$$

This holds, in fact, for all $p \in \mathbb{R}^3$ since the left side is equal to $2K^{0,0} + \frac{1}{2}h^2p^2 + 2E_b$.

By combining (4.15) with (4.13), (4.14) and (4.8) we see that $\|\nabla \psi\|_2$ is bounded by a constant times $\|\psi\|_2$. To conclude the uniform upper bound on the H^1 norm of ψ , it thus suffices to give a bound on the L^2 norm. To do this, we have to utilize the first term on the left side of Eq. (4.8).

Eq. (4.10) states that α can be decomposed as $\alpha = h\alpha_0\psi + \xi_0$, where α_0 is short for the operator $\hat{\alpha}_0(-ih\nabla)$. The following lemma was proved in [6, Lemma 6]. It gives a lower bound on $(\text{Tr}(\alpha\bar{\alpha})^2)^{1/4}$, the 4-norm of α . This bound holds under appropriate decay and smoothness assumptions on α_0 which are satisfied in our case. (See the discussion at the beginning of Section 3.)

Lemma 1. *For some $0 < C < \infty$ we have*

$$\begin{aligned} \|\alpha\|_4 &\geq \left[h \int_{\mathcal{C}} |\psi(x)|^4 dx \int_{\mathbb{R}^3} \widehat{\alpha}_0(q)^4 \frac{dq}{(2\pi)^3} - Ch^2 \|\psi\|_{H^1(\mathcal{C})}^4 \right]_+^{1/4} \\ &\quad - Ch^{1/4} \|\psi\|_2^{1/2} \left(1 + Ch^{1/4} \|\psi\|_4 \right)^{1/2}, \end{aligned} \quad (4.18)$$

where $[\cdot]_+ = \max\{0, \cdot\}$ denotes the positive part.

The fact that $\|\nabla\psi\|_2 \leq C\|\psi\|_2$ also implies that $\|\psi\|_4 \leq C\|\psi\|_2$ via Sobolev's inequality for functions on the torus. If we use also that $\|\psi\|_4 \geq \|\psi\|_2$ we conclude from (4.18) that $\|\alpha\|_4 \geq Ch^{1/4}(\|\psi\|_2 - C\|\psi\|_2^{1/2})$ for h small enough. In combination with (4.8) and (4.13) this implies that $\|\psi\|_2 \leq C$. This shows that the H^1 norm of ψ is indeed uniformly bounded.

It follows that $\|\xi\|_2 \leq O(h^{1/2})$. To conclude the proof of (4.1), we need to show that also $\|\xi\|_{H^1} \leq O(h^{1/2})$. We can write

$$\xi(x, y) = \xi_0(x, y) + \frac{\psi(x) - \psi(y)}{2(2\pi)^{3/2}h^2} \alpha_0(h^{-1}(x - y)). \quad (4.19)$$

From the definition (4.10) it follows easily that $\|\xi_0\|_{H^1} \leq O(h^{1/2})$, using that $-h^2\nabla^2$ is relatively bounded with respect to $K^{0,0} + V(h^{-1}(\cdot - y)) + 1$. If we use the boundedness of the H^1 norm of ψ and, moreover,

$$\begin{aligned} &h^{-3} \int_{\mathcal{C} \times \mathbb{R}^3} |\psi(x) - \psi(y)|^2 |\nabla \alpha_0(h^{-1}(x - y))|^2 dx dy \\ &= 4 \sum_{p \in (2\pi\mathbb{Z})^3} |\widehat{\psi}(p)|^2 \int_{\mathbb{R}^3} |\nabla \alpha_0(x)|^2 \sin^2\left(\frac{1}{2}hp \cdot x\right) dx \leq O(h^2) \end{aligned} \quad (4.20)$$

(since $\int |\nabla \alpha_0|^2 |x|^2 dx$ is finite), the bound on the H^1 norm of ξ readily follows. This completes the proof of Proposition 1. \square

Given Proposition 1, the proof of the lower bound on the ground state energy is very similar to the corresponding one in [6, Sect. 7]. Let Γ be a state with $\mathcal{E}^{\text{BCS}}(\Gamma) \leq 0$, and let ψ be the function defined by the decomposition (4.1). In order to be able to apply Theorems 2 and 3, we have to make sure that ψ is in H^2 . For this purpose, we pick some $\epsilon > 0$ with $h < \epsilon < 1$ and define $\psi_{<}$ via its Fourier coefficients

$$\widehat{\psi}_{<}(p) = \widehat{\psi}(p) \theta(\epsilon h^{-1} - |p|). \quad (4.21)$$

The function $\psi_{<}$ is thus smooth, and $\|\psi_{<}\|_{H^2} \leq C\epsilon h^{-1}$ since ψ is bounded in H^1 .

Let also $\psi_{>} = \psi - \psi_{<}$. Since ψ is bounded in H^1 , the $L^2(\mathcal{C})$ norm of $\psi_{>}$ is bounded by $O(h\epsilon^{-1})$. We absorb the part $\frac{1}{2}(\psi_{>}(x) + \psi_{>}(y))\alpha_0(h^{-1}(x - y))$ into ξ , and write

$$\alpha(x, y) = \frac{\psi_{<}(x) + \psi_{<}(y)}{2(2\pi)^{3/2}h^2} \alpha_0(h^{-1}(x - y)) + \sigma(x, y) \quad (4.22)$$

where

$$\sigma(x, y) = \xi(x, y) + \frac{\psi_{>}(x) + \psi_{>}(y)}{2(2\pi)^{3/2}h^2} \alpha_0(h^{-1}(x - y)). \quad (4.23)$$

Proposition 1 shows that $\|\xi\|_{H^1} \leq O(h^{1/2})$. From the bound $\|\psi_>\|_2 \leq O(h\epsilon^{-1})$ it thus follows that $\|\sigma\|_2 \leq O(h^{1/2}\epsilon^{-1})$. We cannot conclude the same bound for the H^1 norm of σ , however.

As in (2.3), let Δ denote the operator $\Delta = -\frac{1}{2}(\psi_<(x)t(-ih\nabla) + t(-ih\nabla)\psi_<(x))$. The function t is given in (3.1), as in the previous section. Let H_Δ be the corresponding Hamiltonian defined in (2.4). We can write

$$\begin{aligned} \mathcal{E}^{\text{BCS}}(\Gamma) &= -\frac{1}{2} \text{Tr}_0 ([H_\Delta]_- - [H_0]_-) \\ &\quad - \frac{1}{4h^4} \int_{\mathcal{C} \times \mathbb{R}^3} V\left(\frac{x-y}{h}\right) |\psi_<(x) + \psi_<(y)|^2 |\alpha_0\left(\frac{x-y}{h}\right)|^2 \frac{dx dy}{(2\pi)^3} \\ &\quad + \frac{1}{2} \text{Tr}_0 H_\Delta(\Gamma - \Gamma_\Delta) + \int_{\mathcal{C} \times \mathbb{R}^3} V(h^{-1}(x-y)) |\sigma(x, y)|^2 dx dy, \end{aligned} \quad (4.24)$$

where Tr_0 denotes again the sum of the trace per unit volume of the diagonal entries, as in (3.4).

The terms in the first two lines on the right side of (4.24) have already been calculated. The first term is estimated in Theorem 2, and a bound on the second term was derived in Section 3 on the upper bound. Using the fact that the H^1 norm of $\psi_<$ is uniformly bounded, as well as $\|\psi_<\|_{H^2} \leq C\epsilon/h$, we obtain the lower bound

$$\begin{aligned} \mathcal{E}^{\text{BCS}}(\Gamma) &\geq h (\mathcal{E}^{\text{GP}}(\psi_<) - C(h + \epsilon^2)) \\ &\quad + \frac{1}{2} \text{Tr}_0 H_\Delta(\Gamma - \Gamma_\Delta) + \int_{\mathcal{C} \times \mathbb{R}^3} V(h^{-1}(x-y)) |\sigma(x, y)|^2 dx dy. \end{aligned} \quad (4.25)$$

It remains to show that the terms in the last line of (4.25) are negligible, i.e., of higher order than h , for an appropriate choice of $\epsilon \ll 1$. We shall use the following lemma, whose proof is inspired by [11, Lemma 1].

Lemma 2. *For all $0 \leq \Gamma \leq 1$ with $(-\nabla^2 + 1)\gamma$ trace class, we have*

$$\text{Tr}_0 H_\Delta(\Gamma - \Gamma_\Delta) \geq \text{Tr} (\Gamma - \Gamma_\Delta) |H_\Delta| (\Gamma - \Gamma_\Delta). \quad (4.26)$$

Proof. Recall that Γ_Δ is the projection onto the negative spectral subspace of H_Δ . Moreover, for any operator A , $\text{Tr}_0 A = \text{Tr} \Gamma_0 A \Gamma_0 + \text{Tr} (1 - \Gamma_0) A (1 - \Gamma_0)$. A simple calculation shows that

$$\begin{aligned} &\Gamma_0 H_\Delta(\Gamma - \Gamma_\Delta) \Gamma_0 + (1 - \Gamma_0) H_\Delta(\Gamma - \Gamma_\Delta) (1 - \Gamma_0) \\ &= H_\Delta^+ \Gamma (1 - \Gamma_\Delta) + H_\Delta^- (1 - \Gamma) \Gamma_\Delta - E_1 - E_2 \end{aligned} \quad (4.27)$$

with H_Δ^\pm denoting the positive and negative parts of H_Δ , respectively,

$$E_1 = (\Gamma_0 - \Gamma_\Delta) H_\Delta(\Gamma - \Gamma_\Delta) (1 - 2\Gamma_0) \quad (4.28)$$

and

$$E_2 = |H_\Delta| (\Gamma - \Gamma_\Delta) (\Gamma_0 - \Gamma_\Delta). \quad (4.29)$$

It is easy to see that $(\Gamma_0 - \Gamma_\Delta) |H_0|^{1/2}$ and $|H_0|^{1/2} (\Gamma - \Gamma_\Delta)$ are Hilbert-Schmidt; since Δ is bounded, also $(\Gamma_0 - \Gamma_\Delta) |H_\Delta|^{1/2}$ and $|H_\Delta|^{1/2} (\Gamma - \Gamma_\Delta)$ are Hilbert-Schmidt. Hence

E_1 is trace class and, by cyclicity, its trace is equal to the one of

$$\begin{aligned}\tilde{E}_1 &= \sqrt{H_\Delta^+}(\Gamma - \Gamma_\Delta)(1 - 2\Gamma_0)(\Gamma_0 - \Gamma_\Delta)\sqrt{H_\Delta^+} \\ &\quad - \sqrt{H_\Delta^-}(\Gamma - \Gamma_\Delta)(1 - 2\Gamma_0)(\Gamma_0 - \Gamma_\Delta)\sqrt{H_\Delta^-} \\ &= -\sqrt{H_\Delta^+}(\Gamma - \Gamma_\Delta)(\Gamma_0 - \Gamma_\Delta)\sqrt{H_\Delta^+} - \sqrt{H_\Delta^-}(\Gamma - \Gamma_\Delta)(\Gamma_0 - \Gamma_\Delta)\sqrt{H_\Delta^-}. \quad (4.30)\end{aligned}$$

Via the Floquet decomposition, H_Δ can be written as a direct integral of operators on $L^2(\mathcal{C})$ each of which has discrete spectrum. Since we know, a priori, that (4.27) is trace class, we can evaluate the trace in the basis given by H_Δ . With this understanding of the trace, we have $\text{Tr}[\tilde{E}_1 + E_2] = 0$, and thus

$$\begin{aligned}\text{Tr}_0 H_\Delta(\Gamma - \Gamma_\Delta) &= \text{Tr} [H_\Delta^+ \Gamma(1 - \Gamma_\Delta) + H_\Delta^-(1 - \Gamma)\Gamma_\Delta] \\ &= \text{Tr} \left[\sqrt{H_\Delta^+} \Gamma \sqrt{H_\Delta^+} + \sqrt{H_\Delta^-} (1 - \Gamma) \sqrt{H_\Delta^-} \right]. \quad (4.31)\end{aligned}$$

The operators on the last line are positive, hence they are trace class. Estimating $\Gamma \geq \Gamma^2$ and $1 - \Gamma \geq (1 - \Gamma)^2$, respectively, gives the desired bound

$$\begin{aligned}\text{Tr}_0 H_\Delta(\Gamma - \Gamma_\Delta) &\geq \text{Tr} \left[\sqrt{H_\Delta^+} \Gamma^2 \sqrt{H_\Delta^+} + \sqrt{H_\Delta^-} (1 - \Gamma)^2 \sqrt{H_\Delta^-} \right] \\ &= \text{Tr} \left[\sqrt{H_\Delta^+} (\Gamma - \Gamma_\Delta)^2 \sqrt{H_\Delta^+} + \sqrt{H_\Delta^-} (\Gamma - \Gamma_\Delta)^2 \sqrt{H_\Delta^-} \right], \quad (4.32)\end{aligned}$$

which agrees with the right side of (4.26). \square

An application of Schwarz's inequality yields

$$H_\Delta^2 \geq (1 - \eta)H_0^2 - \eta^{-1}\|\Delta\|_\infty^2 \quad (4.33)$$

for any $\eta > 0$. Schwarz's inequality can also be used to obtain a lower bound on H_0^2 . For any $0 < \delta < 1$,

$$\begin{aligned}\left[(-ih\nabla + hA(x))^2 + E_b + h^2W(x) \right]^2 &\geq (1 - \delta)^2 [-h^2\nabla^2 + E_b]^2 \\ &\quad - \frac{1}{\delta} \left[(-ih^2\nabla \cdot A(x) - ih^2A(x) \cdot \nabla)^2 + h^4(W(x) + A(x)^2)^2 \right]. \quad (4.34)\end{aligned}$$

We can further bound

$$\begin{aligned}&(-ih^2\nabla \cdot A(x) - ih^2A(x) \cdot \nabla)^2 \\ &= (-2ih^2\nabla \cdot A(x) + ih^2\text{div} A(x)) (-2ih^2A(x) \cdot \nabla - ih^2\text{div} A(x)) \\ &\leq 8h^4\nabla \cdot A(x)A(x) \cdot \nabla + 2h^4(\text{div} A(x))^2. \quad (4.35)\end{aligned}$$

Since A is C^1 by assumption, this is bounded from above by $Ch^4(-\nabla^2 + 1)$. Choosing $\delta = O(h)$, we thus conclude that

$$H_0^2 \geq (1 - O(h))[-h^2\nabla^2 + E_b]^2 \otimes \mathbb{I}_{\mathbb{C}^2}. \quad (4.36)$$

The operator monotonicity of the square root implies that

$$K^{0,0} \otimes \mathbb{I}_{\mathbb{C}^2} \leq (1 - \eta - O(h))^{-1/2} \sqrt{H_\Delta^2 + \eta^{-1}\|\Delta\|_\infty^2}. \quad (4.37)$$

Using again (4.33) and the fact that $H_0^2 \geq (\lambda^{A,W})^2 \geq O(1)$, the choice $\eta = O(\|\Delta\|_\infty)$ gives

$$|H_\Delta| \geq (1 - O(h + \|\Delta\|_\infty)) K^{0,0} \otimes \mathbb{I}_{\mathbb{C}^2}. \quad (4.38)$$

In particular, we infer from (4.26) that

$$\frac{1}{2} \operatorname{Tr} H_\Delta (\Gamma - \Gamma_\Delta) \geq (1 - O(h + \|\Delta\|_\infty)) \operatorname{Tr} K^{0,0} (\alpha - \alpha_\Delta) (\bar{\alpha} - \bar{\alpha}_\Delta), \quad (4.39)$$

where α_Δ denotes again the upper off-diagonal entry of Γ_Δ . From the definition of Δ , we see that

$$\|\Delta\|_\infty \leq h \|\psi_{<}\|_\infty \|t\|_\infty. \quad (4.40)$$

Moreover, since the Fourier transform of $\psi_{<}$ is supported in the ball $|p| \leq \epsilon/h$,

$$\|\psi_{<}\|_\infty \leq \sum_p |\widehat{\psi_{<}}(p)| \leq \|\psi_{<}\|_{H^1(\mathcal{C})} \left(\sum_{|p| \leq \epsilon h^{-1}} \frac{1}{1+p^2} \right)^{1/2} \leq C \sqrt{\epsilon/h}, \quad (4.41)$$

and hence $\|\Delta\|_\infty \leq O(\epsilon^{1/2} h^{1/2})$.

Recall the decomposition (4.22) of α . We decompose α_Δ in a similar way, and define ϕ by

$$\alpha_\Delta = \frac{h}{2} (\psi_{<}(x) \widehat{\alpha}_0(-ih\nabla) + \widehat{\alpha}_0(-ih\nabla) \psi_{<}(x)) + \phi. \quad (4.42)$$

In particular, we have

$$\alpha - \alpha_\Delta = \sigma - \phi. \quad (4.43)$$

Since $\|\psi_{<}\|_{H^2} \leq O(\epsilon/h)$, Theorem 3 implies that $\|\phi\|_{H^1} \leq O(\epsilon h^{1/2})$. From the positivity of $K^{0,0}$ we conclude that

$$\operatorname{Tr} K^{0,0} (\sigma - \phi) (\bar{\sigma} - \bar{\phi}) \geq \operatorname{Tr} K^{0,0} \sigma \bar{\sigma} - 2 \operatorname{Re} \operatorname{Tr} K^{0,0} \sigma \bar{\phi}. \quad (4.44)$$

The terms quadratic in σ are thus

$$(1 - \delta) \operatorname{Tr} K^{0,0} \sigma \bar{\sigma} + \int_{\mathcal{C} \times \mathbb{R}^3} V(h^{-1}(x - y)) |\sigma(x, y)|^2 dx dy \quad (4.45)$$

with $\delta = O(h + \|\Delta\|_\infty) = O(\epsilon^{1/2} h^{1/2})$. Pick some $\tilde{\delta} \geq 0$ with $\delta + \tilde{\delta} \leq 1/2$, and write

$$\begin{aligned} (1 - \delta) K^{0,0} + V &= \tilde{\delta} K^{0,0} + (1 - 2\delta - 2\tilde{\delta}) (K^{0,0} + V) + (\delta + \tilde{\delta}) (K^{0,0} + 2V) \\ &\geq \tilde{\delta} K^{0,0} - C (\delta + \tilde{\delta}), \end{aligned} \quad (4.46)$$

where we have used that V is relatively form-bounded with respect to $K^{0,0}$ to bound the last term. Hence (4.45) is bounded from below by

$$\tilde{\delta} (\|\sigma\|_{H^1}^2 - (C - E_b + 1) \|\sigma\|_2^2) - C \delta \|\sigma\|_2^2. \quad (4.47)$$

Recall that $\|\sigma\|_2 \leq O(h^{1/2}/\epsilon)$. We shall choose $\tilde{\delta} = 0$ if the first parenthesis on the right side of (4.47) is less than $\frac{1}{2} \|\sigma\|_{H^1}^2$ (and, in particular, if it is negative), while $\tilde{\delta} = O(1)$ in the opposite case, i.e., when $\|\sigma\|_{H^1}^2 \geq 2(C - E_b + 1) \|\sigma\|_2^2$. In the latter case we shall have the positive term $\tilde{\delta} \|\sigma\|_{H^1}^2 / 2$ at our disposal, which will be used in (4.50) below.

We are left with estimating the last term in (4.44), which is linear in σ . Recall from (4.23) that σ is a sum of two terms, ξ and $\sigma - \xi$, where the latter is proportional to $\psi_{>}$, and $\|\xi\|_{H^1} \leq O(h^{1/2})$ independently of ϵ . Moreover, as the proof of Theorem 3

shows, ϕ is the sum of two terms, η_1 and $\phi - \eta_1$, with η_1 defined in (2.14) (with ψ replaced by $\psi_{<}$) and $\|\phi - \eta_1\|_{H^1} \leq O(h^{3/2})$. Now

$$\mathrm{Tr} K^{0,0}(\sigma - \xi) \bar{\eta}_1 = 0 \quad (4.48)$$

as can be seen by writing out the trace in momentum space and using that $\widehat{\psi}_{<}$ and $\widehat{\psi}_{>}$ have disjoint support. Hence

$$\begin{aligned} \mathrm{Re} \mathrm{Tr} K^{0,0} \sigma \bar{\phi} &\leq C (\|\xi\|_{H^1} \|\phi\|_{H^1} + \|\sigma\|_{H^1} \|\phi - \eta_1\|_{H^1}) \\ &\leq O(\epsilon h) + O(h^{3/2}) \|\sigma\|_{H^1}. \end{aligned} \quad (4.49)$$

In the case $\|\sigma\|_{H^1} \leq C\|\sigma\|_2$ (corresponding to $\tilde{\delta} = 0$ above) we can further bound $\|\sigma\|_{H^1} \leq O(h^{1/2}/\epsilon)$. In the opposite case, where $\tilde{\delta} = O(1)$, we can use the positive term $\tilde{\delta}\|\sigma\|_{H^1}^2/2$ from before and bound

$$\frac{\tilde{\delta}}{2} \|\sigma\|_{H^1}^2 - O(h^{3/2}) \|\sigma\|_{H^1} \geq -O(h^3), \quad (4.50)$$

which thus leads to an even better bound.

In combination with (4.25) these bounds show that

$$\mathcal{E}^{\mathrm{BCS}}(\Gamma) \geq h (\mathcal{E}^{\mathrm{GP}}(\psi_{<}) - Ce) \quad (4.51)$$

where

$$e = h + \epsilon^2 + \epsilon + \frac{h}{\epsilon} + \frac{h^{1/2}}{\epsilon^{3/2}}. \quad (4.52)$$

The choice $\epsilon = h^{1/5}$ leads to $e \leq Ch^{1/5}$.

This completes the lower bound to the BCS energy. The statement (1.9) about approximate minimizers follows immediately from (4.51) and (4.22).

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